

David Balcells

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

78 papers	4,213 citations	31 h-index	64 g-index
88 ext. papers	4,557 ext. citations	8.7 avg, IF	5.59 L-index

#	Paper	IF	Citations
78	C-H bond activation in transition metal species from a computational perspective. <i>Chemical Reviews</i> , 2010 , 110, 749-823	68.1	877
77	Highly active and robust Cp* iridium complexes for catalytic water oxidation. <i>Journal of the American Chemical Society</i> , 2009 , 131, 8730-1	16.4	516
76	Half-sandwich iridium complexes for homogeneous water-oxidation catalysis. <i>Journal of the American Chemical Society</i> , 2010 , 132, 16017-29	16.4	468
75	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. <i>Organometallics</i> , 2008 , 27, 2529-2535	3.8	142
74	Mechanistic Study of an Improved Ni Precatalyst for Suzuki-Miyaura Reactions of Aryl Sulfamates: Understanding the Role of Ni(I) Species. <i>Journal of the American Chemical Society</i> , 2017 , 139, 922-936	16.4	102
73	Insight into the efficiency of cinnamyl-supported precatalysts for the Suzuki-Miyaura reaction: observation of Pd(I) dimers with bridging allyl ligands during catalysis. <i>Journal of the American Chemical Society</i> , 2014 , 136, 7300-16	16.4	102
72	Design of a Versatile and Improved Precatalyst Scaffold for Palladium-Catalyzed Cross-Coupling: (β-1-tBu-indenyl)2(ECl)2Pd2. <i>ACS Catalysis</i> , 2015 , 5, 3680-3688	13.1	101
71	Computational approaches to asymmetric synthesis. <i>New Journal of Chemistry</i> , 2007 , 31, 333	3.6	99
70	An Experimental/Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. <i>Organometallics</i> , 2010 , 29, 6548-6558	3.8	98
69	Manganese catalysts for C-H activation: an experimental/theoretical study identifies the stereoelectronic factor that controls the switch between hydroxylation and desaturation pathways. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7605-16	16.4	94
68	A rational basis for the axial ligand effect in C-H oxidation by [MnO(porphyrin)(X)] ⁺ (X = H ₂ O, OH ⁻ , O ₂ ⁻) from a DFT study. <i>Inorganic Chemistry</i> , 2008 , 47, 10090-9	5.1	84
67	Cp* Iridium Precatalysts for Selective C-H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. <i>ACS Catalysis</i> , 2012 , 2, 208-218	13.1	78
66	Understanding Precatalyst Activation in Cross-Coupling Reactions: Alcohol Facilitated Reduction from Pd(II) to Pd(0) in Precatalysts of the Type (β-allyl)Pd(L)(Cl) and (β-indenyl)Pd(L)(Cl). <i>ACS Catalysis</i> , 2015 , 5, 5596-5606	13.1	76
65	Computational rationalization of the dependence of the enantioselectivity on the nature of the catalyst in the vanadium-catalyzed oxidation of sulfides by hydrogen peroxide. <i>Journal of the American Chemical Society</i> , 2005 , 127, 3624-34	16.4	68
64	Introducing copper as catalyst for oxidative alkane dehydrogenation. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3887-96	16.4	66
63	The rebound mechanism in catalytic C-H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. <i>Chemical Communications</i> , 2008 , 744-6	5.8	64
62	Designing Pd and Ni Catalysts for Cross-Coupling Reactions by Minimizing Off-Cycle Species. <i>ACS Catalysis</i> , 2018 , 8, 3499-3515	13.1	58

61	Nickel(I) monomers and dimers with cyclopentadienyl and indenyl ligands. <i>Chemistry - A European Journal</i> , 2014 , 20, 5327-37	4.8	57
60	Generation and structural characterization of a gold(III) alkene complex. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 1660-3	16.4	56
59	Density functional study on the mechanism of the vanadium-catalyzed oxidation of sulfides by hydrogen peroxide. <i>Journal of Organic Chemistry</i> , 2003 , 68, 4265-74	4.2	55
58	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. <i>Chemical Science</i> , 2020 , 11, 4584-4601	9.4	47
57	C-H oxidation by hydroxo manganese(v) porphyrins: a DFT study. <i>Chemical Communications</i> , 2009 , 1772-4	4.8	41
56	Basic ancillary ligands promote O-O bond formation in iridium-catalyzed water oxidation: a DFT study. <i>Dalton Transactions</i> , 2011 , 40, 11241-7	4.3	40
55	Mechanism of the base-assisted displacement of chloride by alcohol in sulfinyl derivatives. <i>Journal of Organic Chemistry</i> , 2006 , 71, 6388-96	4.2	39
54	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. <i>ACS Catalysis</i> , 2018 , 8, 8751-8762	13.1	38
53	A carbene-rich but carbonyl-poor [Ir ₆ (Ime) ₈ (CO) ₂ H ₁₄](2+) polyhydride cluster as a deactivation product from catalytic glycerol dehydrogenation. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 12808-11	16.4	37
52	Experimental and computational studies of borohydride catalyzed hydrosilylation of a variety of CO and CN functionalities including esters, amides and heteroarenes. <i>New Journal of Chemistry</i> , 2014 , 38, 1694-1700	3.6	34
51	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9672-9683	16.4	34
50	Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzuki-Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers. <i>Organometallics</i> , 2015 , 34, 381-394	3.8	33
49	High Oxidation State Iridium Mono-oxo Dimers Related to Water Oxidation Catalysis. <i>Journal of the American Chemical Society</i> , 2016 , 138, 15917-15926	16.4	31
48	Atom economic synthesis of amides via transition metal catalyzed rearrangement of oxaziridines. <i>Green Chemistry</i> , 2007 , 9, 976	10	31
47	Polyene Cyclization by a Double Intramolecular Heck Reaction. A DFT Study. <i>Organometallics</i> , 2004 , 23, 2784-2796	3.8	31
46	Dinitrogen-Facilitated Reversible Formation of a SiH Bond in a Pincer-Supported Ni Complex. <i>Organometallics</i> , 2016 , 35, 3154-3162	3.8	30
45	trans-Mutation at Gold(III): A Mechanistic Study of a Catalytic Acetylene Functionalization via a Double Insertion Pathway. <i>ACS Catalysis</i> , 2017 , 7, 5023-5034	13.1	28
44	Molecular recognition in Mn-catalyzed C-H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. <i>Dalton Transactions</i> , 2009 , 5989-6000	4.3	25

43	Some critical issues in the application of quantum mechanics/molecular mechanics methods to the study of transition metal complexes. <i>Faraday Discussions</i> , 2003 , 124, 429-41; discussion 443-55	3.6	25
42	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. <i>Accounts of Chemical Research</i> , 2016 , 49, 1070-8	24.3	25
41	Generation and Structural Characterization of a Gold(III) Alkene Complex. <i>Angewandte Chemie</i> , 2013 , 125, 1704-1707	3.6	24
40	Understanding the Solution and Solid-State Structures of Pd and Pt PSiP Pincer-Supported Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 11411-22	5.1	23
39	tmQM Dataset-Quantum Geometries and Properties of 86k Transition Metal Complexes. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 6135-6146	6.1	21
38	A competing, dual mechanism for catalytic direct benzene hydroxylation from combined experimental-DFT studies. <i>Chemical Science</i> , 2017 , 8, 8373-8383	9.4	19
37	Gel-assisted crystallization of [Ir ₄ (Ime) ₇ (CO)H ₁₀](2+) and [Ir ₄ (Ime) ₈ H ₉](3+) clusters derived from catalytic glycerol dehydrogenation. <i>Dalton Transactions</i> , 2015 , 44, 18403-10	4.3	18
36	Coordination and insertion of alkenes and alkynes in Au(III) complexes: nature of the intermediates from a computational perspective. <i>Dalton Transactions</i> , 2016 , 45, 5504-13	4.3	18
35	Influence of a "Dangling" Co(II) Ion Bound to a [MnCoO] Oxo Cubane. <i>Journal of the American Chemical Society</i> , 2018 , 140, 9030-9033	16.4	18
34	Base-catalyzed inversion of chiral sulfur centers. A computational study. <i>Organic Letters</i> , 2004 , 6, 2197-260	26.0	18
33	Does the metal protect the ancillary ligands? C-H strengthening and deactivation in amines and phosphines upon metal-binding. <i>Chemical Communications</i> , 2014 , 50, 614-6	5.8	16
32	How does the Achiral Base Decide the Stereochemical Outcome in the Dynamic Kinetic Resolution of Sulfinyl Chlorides? A Computational Study. <i>Advanced Synthesis and Catalysis</i> , 2007 , 349, 2103-2110	5.6	16
31	Bis(dialkylphosphino)ferrocene-Ligated Nickel(II) Precatalysts for Suzuki-Miyaura Reactions of Aryl Carbonates. <i>Organometallics</i> , 2019 , 38, 3377-3387	3.8	15
30	Synthetic and Computational Studies on the Rhodium-Catalyzed Hydroamination of Aminoalkenes. <i>ACS Catalysis</i> , 2016 , 6, 5651-5665	13.1	15
29	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 13047-13051	16.4	15
28	An oscillating C ₂ (2-) unit inside a copper rectangle. <i>Chemical Communications</i> , 2003 , 1260-1	5.8	15
27	Small-molecule activation at Au(III): metallacycle construction from ethylene, water, and acetonitrile. <i>Dalton Transactions</i> , 2016 , 45, 14719-24	4.3	13
26	A Dinuclear Iridium(V,V) Oxo-Bridged Complex Characterized Using a Bulk Electrolysis Technique for Crystallizing Highly Oxidizing Compounds. <i>Inorganic Chemistry</i> , 2018 , 57, 5684-5691	5.1	12

25	Isolation and Study of Ruthenium-Cobalt Oxo Cubanes Bearing a High-Valent, Terminal Ru-Oxo with Significant Oxo Radical Character. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19859-19869	16.4	12
24	A Carbene-Rich but Carbonyl-Poor [Ir ₆ (IMe) ₈ (CO) ₂ H ₁₄] ₂ ⁺ Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. <i>Angewandte Chemie</i> , 2014 , 126, 13022-13025	3.6	9
23	DFT Investigation of Suzuki-Miyaura Reactions with Aryl Sulfamates Using a Dialkylbiarylphosphine-Ligated Palladium Catalyst. <i>Organometallics</i> , 2017 , 36, 3664-3675	3.8	9
22	Rational selection of co-catalysts for the deaminative hydrogenation of amides. <i>Chemical Science</i> , 2020 , 11, 2225-2230	9.4	8
21	Quantum chemical modeling of the reaction path of chorismate mutase based on the experimental substrate/product complex. <i>FEBS Open Bio</i> , 2017 , 7, 789-797	2.7	7
20	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. <i>Angewandte Chemie</i> , 2017 , 129, 13227-13231	3.6	7
19	Concerted Proton-Electron Transfer Reactivity at a Multimetallic CoO Cubane Cluster. <i>Inorganic Chemistry</i> , 2020 , 59, 15553-15560	5.1	7
18	Rhodium Complexes Promoting C-O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. <i>Chemistry - A European Journal</i> , 2017 , 23, 5232-5243	4.8	6
17	The neutron diffraction structure of [Ir ₄ (IMe) ₈ H ₁₀] ₂ ⁺ polyhydride cluster: Testing the computational hydride positional assignments. <i>Journal of Organometallic Chemistry</i> , 2017 , 849-850, 17-21	2.3	6
16	Synthesis and Characterization of Stable Gold(III) PNP Pincer Complexes. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 3113-3117	2.3	6
15	Cyclometalated ruthenium complexes with carboxylated ligands from a combined experimental/computational perspective. <i>Dalton Transactions</i> , 2018 , 47, 2589-2601	4.3	6
14	Self-Consistency versus Best-Fit Approaches in Understanding the Structure of Metal Nitrosyl Complexes. <i>Organometallics</i> , 2004 , 23, 6008-6014	3.8	4
13	C-H Activation by RuCoO Oxo Cubanes: Effects of Oxo Radical Character and Metal-Metal Cooperativity. <i>Journal of the American Chemical Society</i> , 2021 , 143, 12108-12119	16.4	4
12	First-Principles Calculation of H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. <i>Inorganic Chemistry</i> , 2020 , 59, 17509-17518	5.1	3
11	Synthesis, Characterization, and Reactivity of Cyclometalated Gold(III) Dihalide Complexes in Aqua Regia. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 3249-3258	2.3	3
10	Unsymmetrical Naphthyridine-Based Dicopper(I) Complexes: Synthesis, Stability, and Carbon-Hydrogen Bond Activations. <i>Organometallics</i> , 2021 , 40, 1866-1873	3.8	3
9	Synthesis of Triarylmethanes via Palladium-Catalyzed Suzuki-Miyaura Reactions of Diarylmethyl Esters. <i>Organometallics</i> , 2021 , 40, 2332-2344	3.8	2
8	A Career in Catalysis: Odile Eisenstein. <i>ACS Catalysis</i> , 2019 , 9, 10375-10388	13.1	1

7	Distortional Effects of Noncovalent Interactions in the Crystal Lattice of a Cp*Ir(III) Acylhydroxamic Acid Complex: A Joint Experimental/Computational Study. <i>Organometallics</i> , 2014 , 33, 4417-4424	3.8	1
6	A DFT Perspective on Diels-Alder Organocatalysts Based on Substituted Phosphoramides. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 442-450	3.2	1
5	Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane C-H Activation Transition States. <i>Topics in Catalysis</i> , 1	2.3	1
4	Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. <i>RSC Advances</i> , 2014 , 4, 24729-24735	3.7	0
3	Computational Studies on Asymmetric Reactions with Sulfur Reagents	399-416	0
2	Concerted Cycloaddition Mechanism in the CuAAC Reaction Catalyzed by 1,8-Naphthyridine Dicopper Complexes. <i>ACS Catalysis</i> , 4744-4753	13.1	0
1	Computational Studies on the Mechanisms for Deaminative Amide Hydrogenation by Homogeneous Bifunctional Catalysts. <i>Topics in Catalysis</i> , 2022 , 65, 82-95	2.3	0